Claims

What is claimed is:

1. A method for spatially profiling proteins, the method comprising the steps of:

determining a hydrophobicity distribution of a protein; and

shifting the hydrophobicity distribution.

2. The method of claim 1, wherein the step of shifting the hydrophobicity distribution comprises the step of shifting the hydrophobicity distribution such that a total hydrophobicity of the protein is zero.

3. The method of claim 2, further comprising the step of normalizing the shifted hydrophobicity distribution, thereby causing a standard deviation of the shifted hydrophobicity distribution to be unity.

4. The method of claim 3, further comprising the steps of:

determining, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

determining a profile of the adjusted zero-order moment of hydrophobicity;

determining a first distance of a maximum peak of a profile of the adjusted zero-order moment of hydrophobicity;

determining a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

determining a ratio between the first and second distances.

5. The method of claim 3, further comprising the steps of:

determining, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity;

determining a profile of the adjusted second-order moment of hydrophobicity;

determining a first distance at which a maximum peak of the profile of the adjusted second-order moment of hydrophobicity occurs;

determining, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

determining a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

determining a ratio between the first and second distances.

6. The method of claim 1, wherein the step of determining a hydrophobicity distribution of a protein comprises the step of assigning a hydrophobicity value to each of a plurality of residues of the protein.

7. A method for spatially profiling proteins, the method comprising the steps of:

a) determining a shifted and normalized hydrophobicity distribution for a protein;

b) determining a centroid of the protein;

c) determining, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity; and

d) determining a profile of the adjusted second-order moment of hydrophobicity.

8. The method of claim 7, wherein:

the step of determining a shifted and normalized hydrophobicity distribution comprises the steps of:

I) determining a residue center for each of a plurality of residues of the protein;

II) assigning each residue a hydrophobicity value, where a hydrophobicity value is assigned to a corresponding one of the residue centers;

III) shifting each the hydrophobicity values of the hydrophobicity distribution such that a total hydrophobicity of the protein is zero; and

IV) normalizing each of the hydrophobicity values, wherein the hydrophobicity distribution comprises the shifted and normalized hydrophobicity values, which thereby causes a standard deviation of the hydrophobicity distribution to be unity.

9. The method of claim 7, wherein the step of determining a profile of the adjusted second-order moment of hydrophobicity comprises the step of determining a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero.

10. The method of claim 9, further comprising the steps of:

e) determining, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

f) determining a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is zero; and

g) determining a ratio between the first distance and the second distance.

11. The method of claim 10, wherein:

the step of a determining a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero comprises the step of determining a surface enclosing an interior volume wherein any larger of a surface will yield a negative adjusted second-order moment of hydrophobicity; and

the step of determining a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is zero comprises the step of increasing the volume enclosed by the surface until the net hydrophobicity of the protein is zero.

12. The method of claim 11, wherein the surface is chosen from the group consisting of an ellipsoid and a sphere.

13. The method of claim 10, wherein both the first and second distances describe a surface.

14. The method of claim 13, wherein the surface is chosen from the group consisting of an ellipsoid and a sphere.

15. The method of claim 7, wherein the step of profiling an adjusted second-order moment of hydrophobicity further comprises the step of determining a profile of the adjusted second-order moment of hydrophobicity with distance from the centroid.

16. The method of claim 7, wherein the step of determining a centroid of the protein comprises the steps of:

I) determining a residue center for each of a plurality of residues of the protein;

II) assigning each of the residue centers a mass value of one; and

III) determining a center of mass of the protein by using the residue centers and the mass value of one at each residue centroid.

17. The method of claim 16, wherein the step of determining a residue center comprises, for each residue in the protein:

A) determining a location of each atom in the residue;

B) assigning a mass value of one to each location; and

C) determining a center of mass of the residue by using the locations of each atom and the mass value of one at each location;

18. The method of claim 16, wherein the step of determining a residue center comprises, for each residue in the protein, determining an alpha carbon atom location.

19. A method for spatially profiling proteins, the method comprising the steps of:

determining a shifted and normalized hydrophobicity distribution for a protein;

determining a centroid of the protein;

selecting a surface; and

calculating, by using the surface, a moment of the shifted and normalized hydrophobicity distribution.

20. The method of claim 19., wherein the moment is selected from the group consisting of a zero-order moment and a second-order moment.

21. The method of claim 19, wherein the surface is selected from the group consisting of a sphere and an ellipse.

22. A system comprising:

a memory that stores computer-readable code; and

a processor operatively coupled to the memory, the processor configured to implement the computer-readable code, the computer-readable code configured to:

determine a hydrophobicity distribution of a protein; and

shift the hydrophobicity distribution.

23. The system of claim 22, wherein the computer-readable code is further configured, when shifting the hydrophobicity distribution, to shift the hydrophobicity distribution such that a total hydrophobicity of the protein is zero.

24. The system of claim 23, wherein the computer-readable code is further configured to normalize the shifted hydrophobicity distribution, thereby causing a standard deviation of the shifted hydrophobicity distribution to be unity.

25. The system of claim 24, wherein the computer-readable code is further configured to:

determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

determine a profile of the adjusted zero-order moment of hydrophobicity;

determine a first distance of a maximum peak of a profile of the adjusted zero-order moment of hydrophobicity;

determine a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

determine a ratio between the first and second distances.

26. The system of claim 24, wherein the computer-readable code is further configured to:

determine, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity;

determine a profile of the adjusted second-order moment of hydrophobicity;

determine a first distance at which a maximum peak of the profile of the adjusted second-order moment of hydrophobicity occurs;

determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

determine a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

determine a ratio between the first and second distances.

27. The system of claim 22, wherein the computer-readable code is further configured, when determining a hydrophobicity distribution of a protein, to assign a hydrophobicity value to each of a plurality of residues of the protein.

28. A system for spatially profiling proteins, comprising:

a memory that stores computer-readable code; and

a processor operatively coupled to the memory, the processor configured to implement the computer-readable code, the computer-readable code configured to:

a) determine a shifted and normalized hydrophobicity distribution for a protein;

b) determine a centroid of the protein;

c) determine, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity; and

d) determine a profile of the adjusted second-order moment of hydrophobicity.

29. The system of claim 28, wherein the computer-readable code is further configured, when determining a profile of the adjusted second-order moment of hydrophobicity, to determine a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero.

30. The system of claim 29, wherein the computer-readable code is further configured to:

e) determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

f) determine a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is zero; and

g) determine a ratio between the first distance and the second distance.

31. The system of claim 30, wherein:

the computer-readable code is further configured, when determining a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero, to determine a surface enclosing an interior volume wherein any larger of a surface will yield a negative adjusted second-order moment of hydrophobicity; and

the computer-readable code is further configured, when determining a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is zero, to increase the volume enclosed by the surface until the net

hydrophobicity of the protein is zero.

32. The system of claim 31, wherein the surface is chosen from the group consisting of an ellipsoid and a sphere.

33. An article of manufacture comprising:

a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a step to determine a hydrophobicity distribution of a protein; and

a step to shift the hydrophobicity distribution.

34. The article of manufacture of claim 33, wherein the computer-readable code further comprises, when shifting the hydrophobicity distribution, a step to shift the hydrophobicity distribution such that a total hydrophobicity of the protein is zero.

35. The article of manufacture of claim 34, wherein the computer-readable code further comprises a step to normalize the shifted hydrophobicity distribution, thereby causing a standard deviation of the shifted hydrophobicity distribution to be unity.

36. The article of manufacture of claim 35, wherein the computer-readable further comprises:

a step to determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

a step to determine a profile of the adjusted zero-order moment of hydrophobicity;

a step to determine a first distance of a maximum peak of a profile of the adjusted zero-order moment of hydrophobicity;

a step to determine a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

a step to determine a ratio between the first and second distances.

37. The article of manufacture of claim 35, wherein the computer-readable code further comprises:

a step to determine, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity;

a step to determine a profile of the adjusted second-order moment of hydrophobicity;

a step to determine a first distance at which a maximum peak of the profile of the adjusted second-order moment of hydrophobicity occurs;

a step to determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

a step to determine a second distance at which the adjusted zero-order moment of hydrophobicity vanishes; and

a step to determine a ratio between the first and second distances.

38. The article of manufacture of claim 33, wherein the computer-readable code further comprises, when determining a hydrophobicity distribution of a protein, a step to assign a hydrophobicity value to each of a plurality of residues of the protein.

39. An article of manufacture for spatially profiling proteins, comprising:

a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a) a step to determine a shifted and normalized hydrophobicity distribution for a protein;

b) a step to determine a centroid of the protein;

c) a step to determine, by using the shifted and normalized hydrophobicity distribution, an adjusted second-order moment of hydrophobicity; and

d) a step to determine a profile of the adjusted second-order moment of hydrophobicity.

40. The article of manufacture of claim 39, wherein the computer-readable code further comprises, when determining a profile of the adjusted second-order moment of hydrophobicity, a step to determine a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero.

41. The article of manufacture of claim 40, wherein the computer-readable code further comprises:

e) a step to determine, by using the shifted and normalized hydrophobicity distribution, an adjusted zero-order moment of hydrophobicity;

f) a step to determine a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is zero; and

g) a step to determine a ratio between the first distance and the second distance.

42. The article of manufacture of claim 41, wherein:

the computer-readable code further comprises, when determining a first distance from the centroid at which the adjusted second-order moment of hydrophobicity is zero, a step to determine a surface enclosing an interior volume wherein any larger of a surface will yield a negative adjusted second-order moment of hydrophobicity; and

the computer-readable code further comprises, when determining a second distance from the centroid at which the adjusted zero-order moment of hydrophobicity is

zero, a step to increase the volume enclosed by the surface until the net hydrophobicity of the protein is zero.

43. The article of manufacture of claim 42, wherein the surface is chosen from the group consisting of an ellipsoid and a sphere.